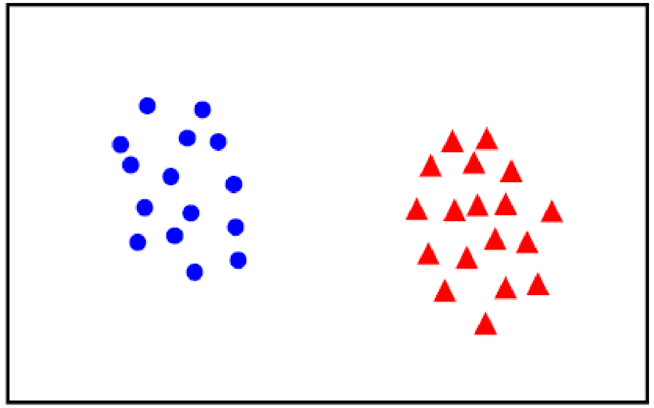
Perceptron
&
Support Vector Machines

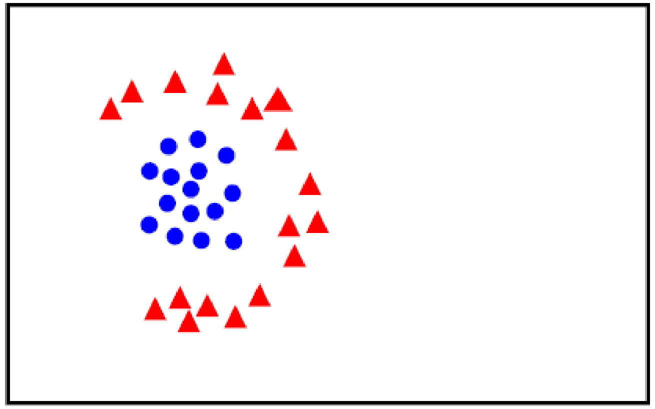
Binary Classification

Given training data $(\mathbf{x}_i, y_i)$ for $i = 1 \ldots N$, with $\mathbf{x}_i \in \mathbb{R}^d$ and $y_i \in \{-1, 1\}$, learn a classifier $f(\mathbf{x})$ such that

$$f(\mathbf{x}_i) \begin{cases} \geq 0 & y_i = +1 \\ < 0 & y_i = -1 \end{cases}$$

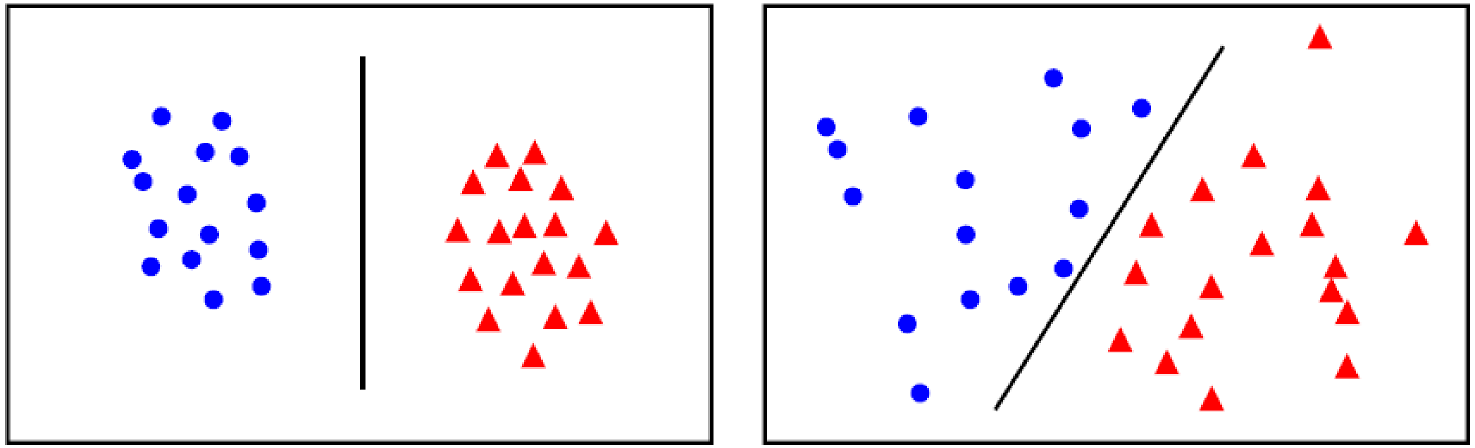
i.e. $y_i f(\mathbf{x}_i) > 0$ for a correct classification.



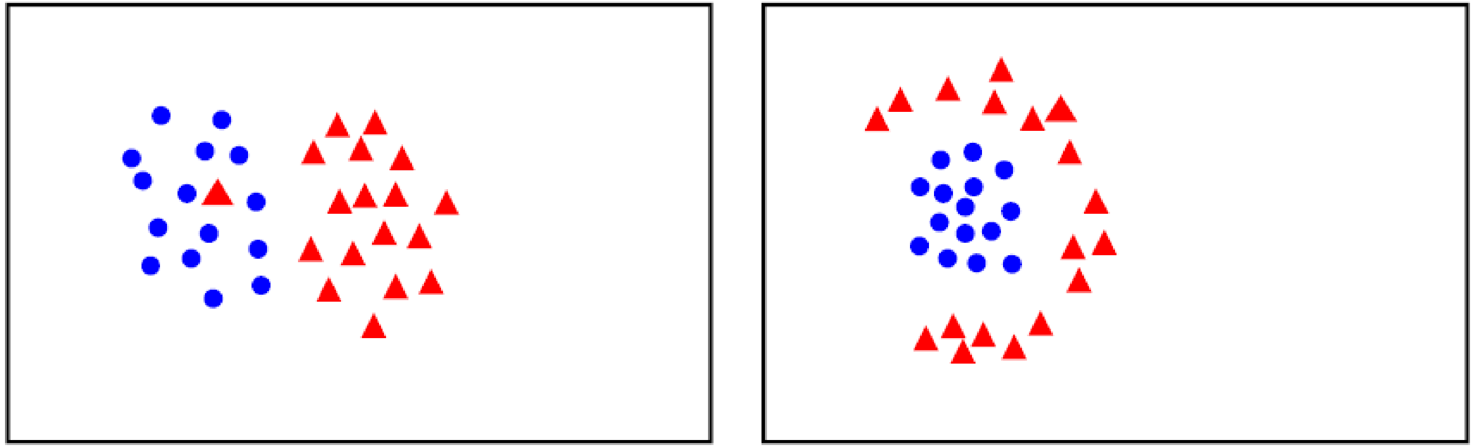


Linear separability

linearly separable



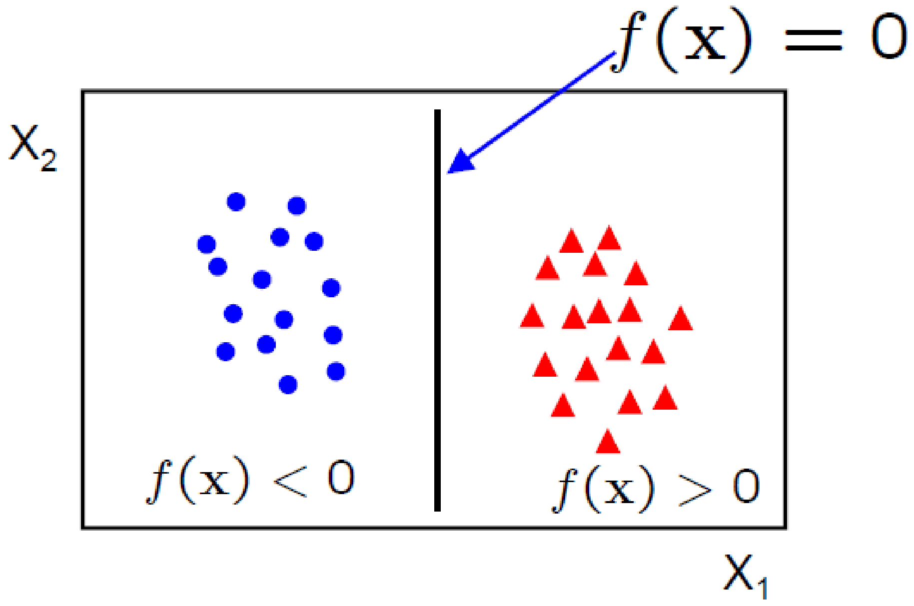
not linearly separable



Linear classifiers

A linear classifier has the form

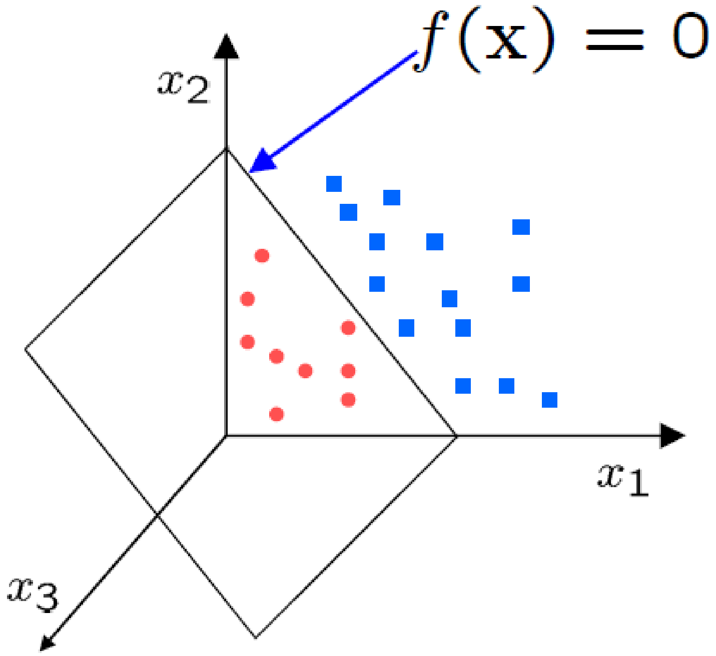
$$f(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + b$$



- in 2D the discriminant is a line
- $\mathbf{w}$ is the normal to the line, and b the bias
- $\mathbf{w}$ is known as the weight vector

Linear classifiers

A linear classifier has the form



$$f(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + b$$

- in 3D the discriminant is a plane, and in nD it is a hyperplane

For a K-NN classifier it was necessary to `carry' the training data

For a linear classifier, the training data is used to learn **w** and then discarded

Only **w** is needed for classifying new data

The Perceptron Classifier

Given linearly separable data $\mathbf{x}_i$ labelled into two categories $y_i = \{-1,1\}$, find a weight vector **w** such that the discriminant function

$$f(\mathbf{x}_i) = \mathbf{w}^\top \mathbf{x}_i + b$$

separates the categories for i = 1, .., N

- how can we find this separating hyperplane ?

The Perceptron Algorithm

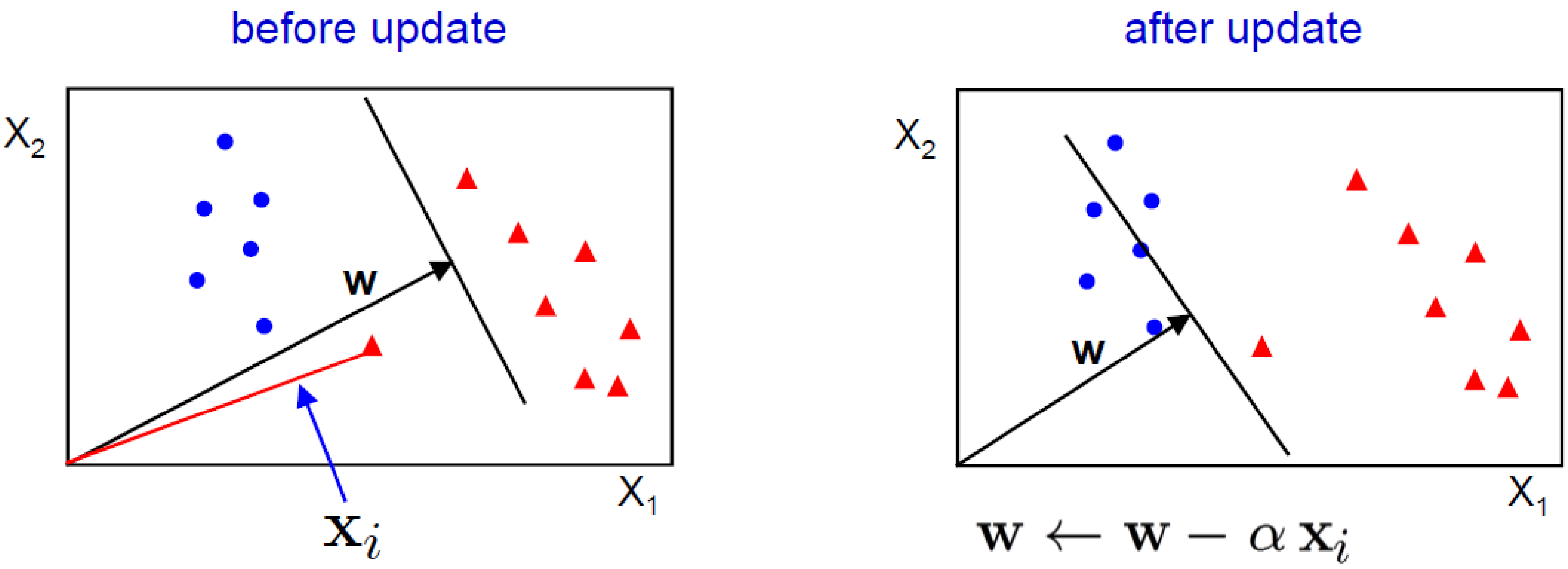
Write classifier as $f(\mathbf{x}_i) = \tilde{\mathbf{w}}^\top \tilde{\mathbf{x}}_i + w_0 = \mathbf{w}^\top \mathbf{x}_i$

where $\mathbf{w} = (\tilde{\mathbf{w}}, w_0), \mathbf{x}_i = (\tilde{\mathbf{x}}_i, 1)$

- Initialize **w** = 0
- Cycle though the data points { $\mathbf{x}_i$, y_i }
  - if $\mathbf{x}_i$ is misclassified then $\mathbf{w} \leftarrow \mathbf{w} + \alpha\, \mathrm{sign}(f(\mathbf{x}_i))\, \mathbf{x}_i$
- Until all the data is correctly classified

For example in 2D

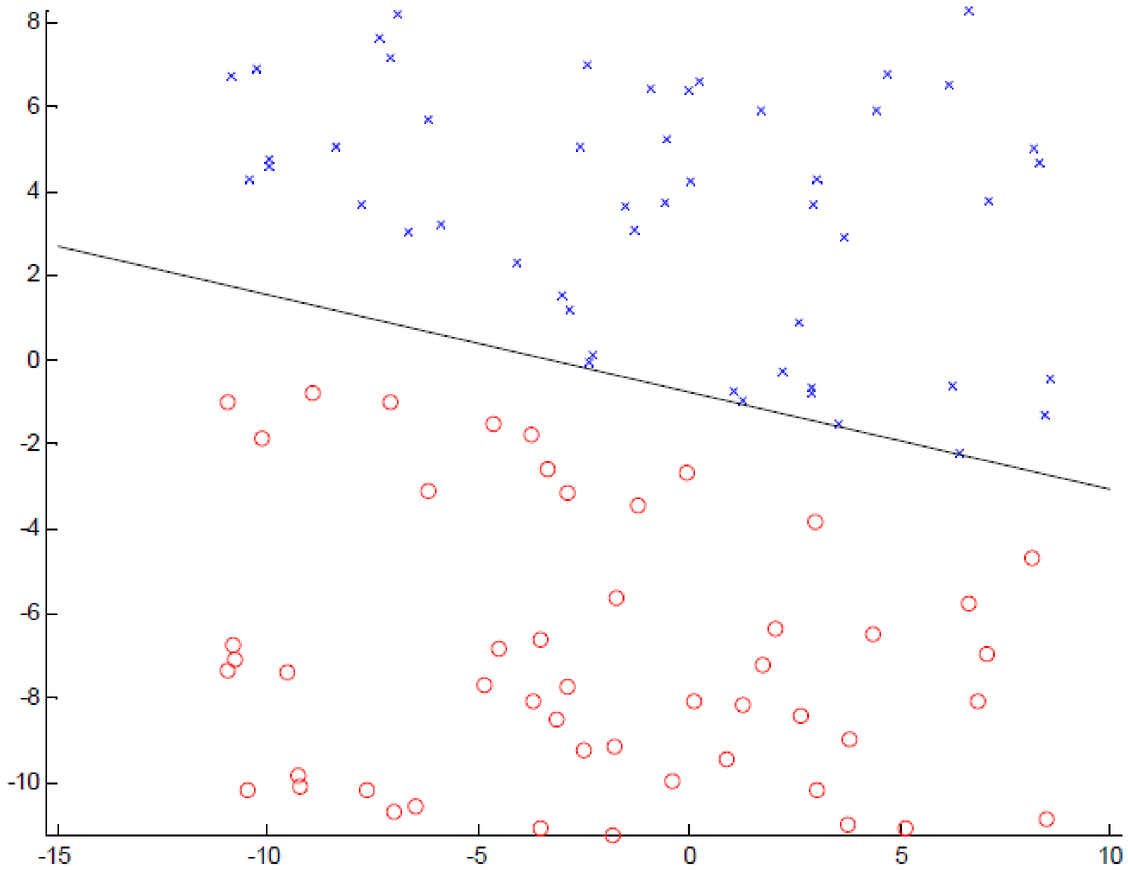
- Initialize **w** = 0
- Cycle though the data points { $\mathbf{x}_i$, y_i }
  - if $\mathbf{x}_i$ is misclassified then $\mathbf{w} \leftarrow \mathbf{w} + \alpha\, \mathrm{sign}(f(\mathbf{x}_i))\, \mathbf{x}_i$
- Until all the data is correctly classified



after convergence $\boxed{\mathbf{w} = \sum_i^N \alpha_i \mathbf{x}_i}$

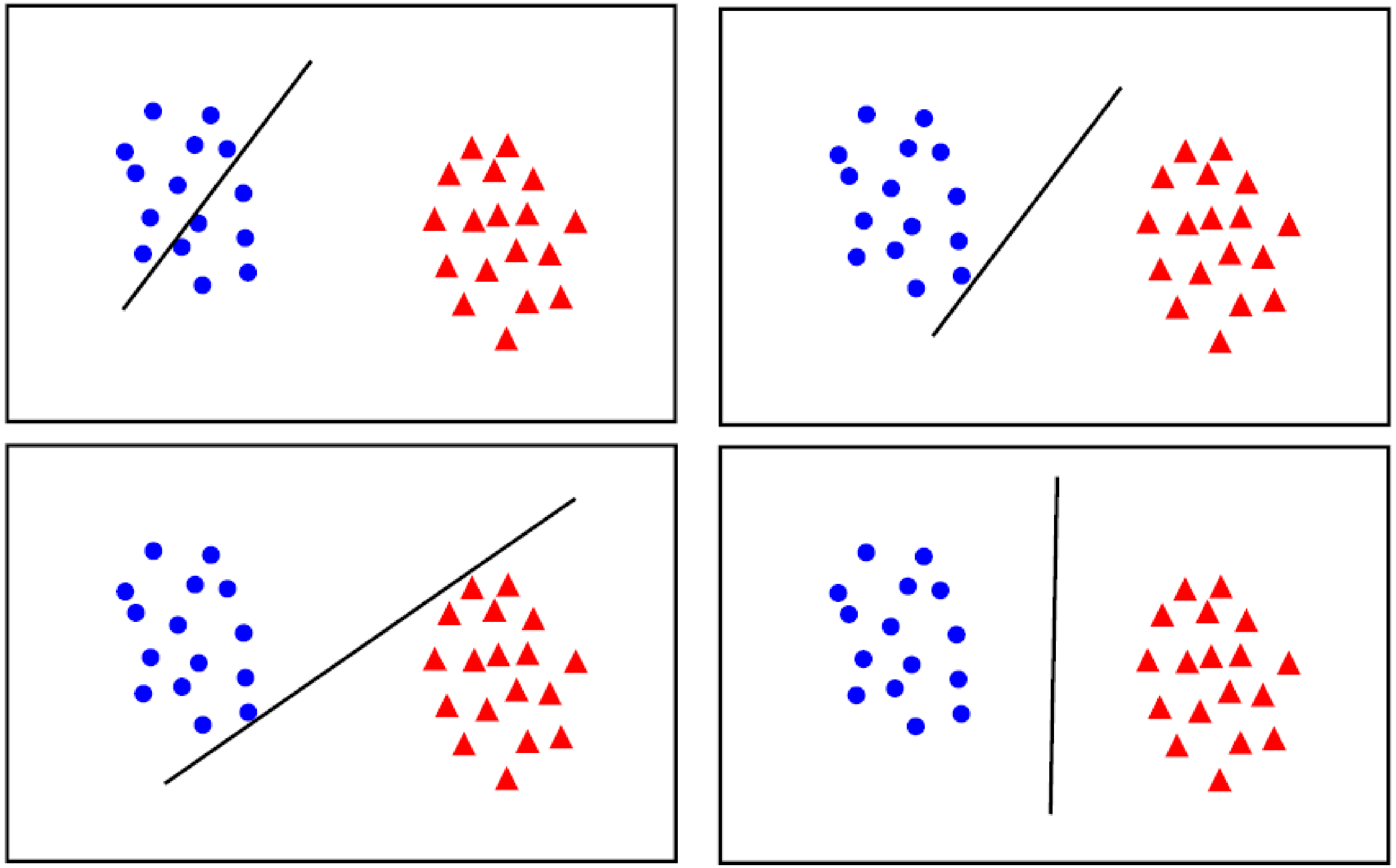
Important!
w is a linear combination of data samples $\mathbf{x}_i$

Perceptron example



- if the data is linearly separable, then the algorithm will converge
- convergence can be slow …
- separating line close to training data
- we would prefer a larger margin for generalization

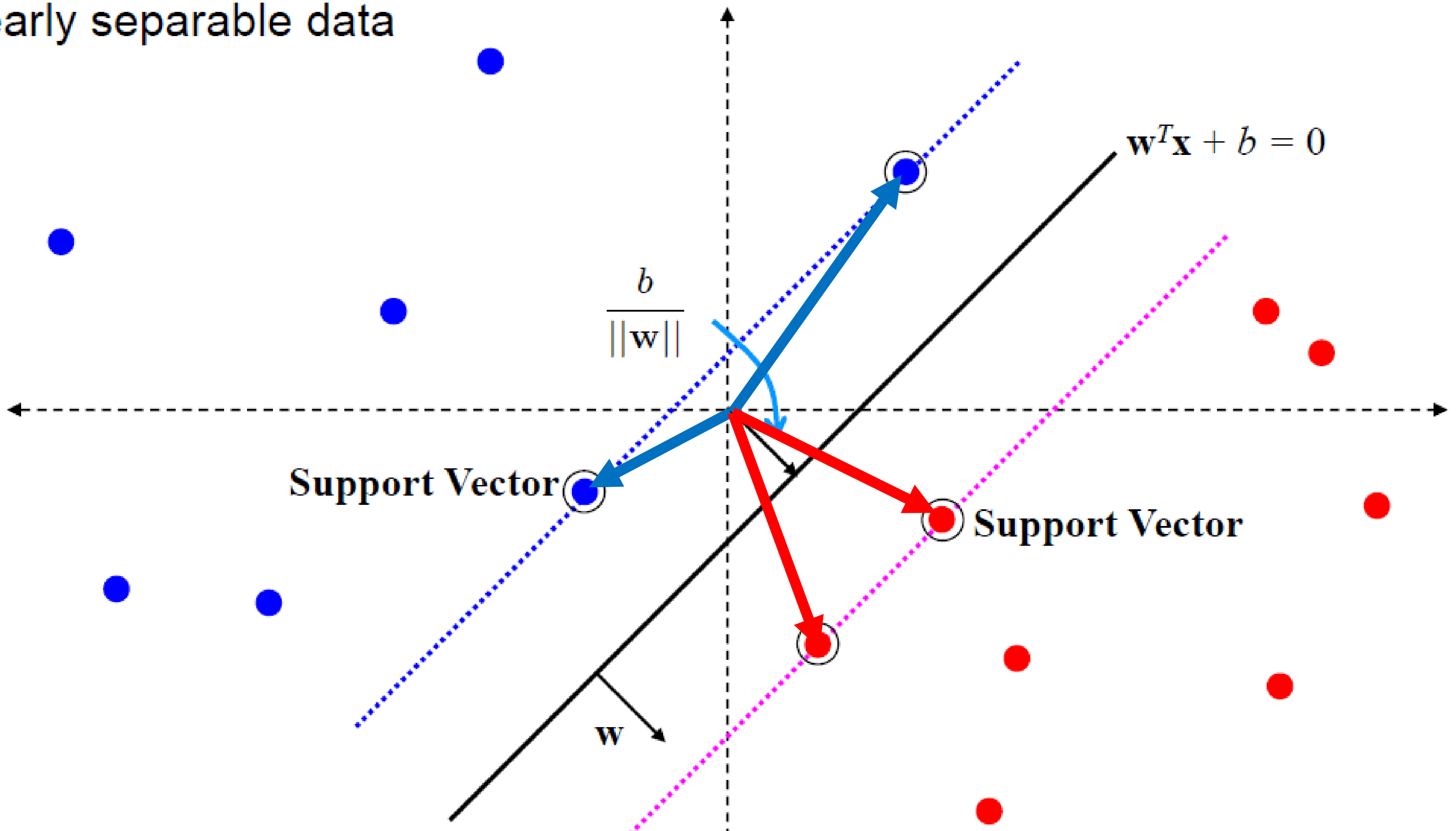
What is the best w?



- maximum margin solution: most stable under perturbations of the inputs

Support Vector Machine

linearly separable data



Support Vectors (intuitive defn.): Points closest to the decision boundary, along the normal **w**

$$f(x) = \sum_i \alpha_i y_i (\boxed{\mathbf{x}_i{}^\top \mathbf{x}}) + b$$

support vectors

Important representation!!

SVM – sketch derivation

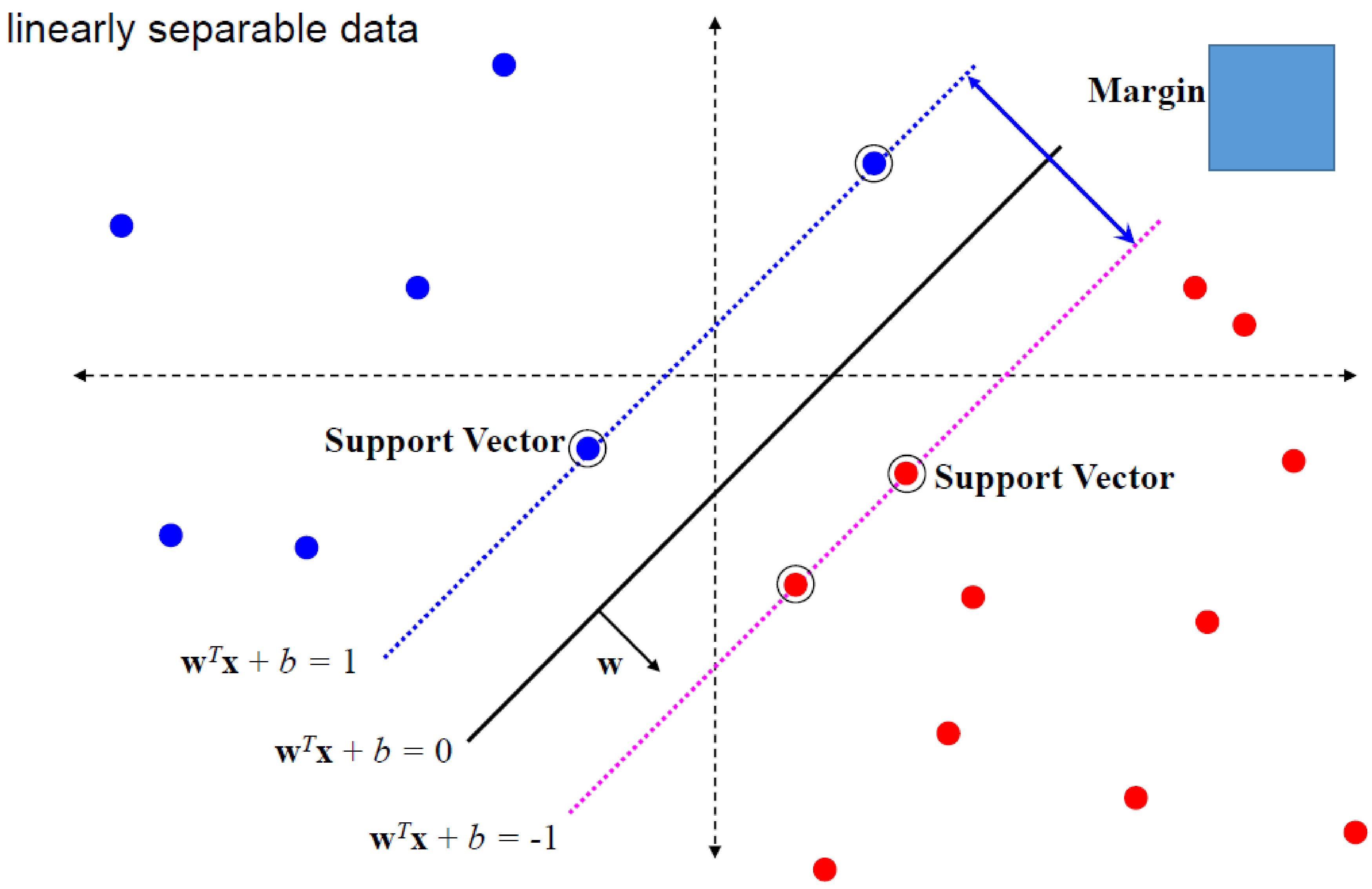
- Since $\mathbf{w}^\top \mathbf{x} + b = 0$ and $c(\mathbf{w}^\top \mathbf{x} + b) = 0$ define the same plane, we have the freedom to choose the normalization of $\mathbf{w}$

- Choose normalization such that $\mathbf{w}^\top \mathbf{x}_+ + b = +1$ and $\mathbf{w}^\top \mathbf{x}_- + b = -1$ for the positive and negative support vectors respectively

- Then the margin is given by

$$\frac{\mathbf{w}}{||\mathbf{w}||} \cdot \left(\mathbf{x}_+ - \mathbf{x}_-\right) = \frac{\mathbf{w}^\top \left(\mathbf{x}_+ - \mathbf{x}_-\right)}{||\mathbf{w}||} = \frac{2}{||\mathbf{w}||}$$

Support Vector Machine



SVM – Optimization

- Learning the SVM can be formulated as an optimization:

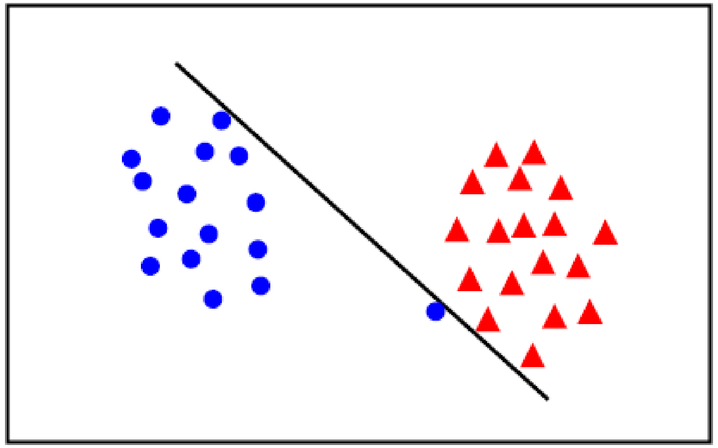
$$\max_{\mathbf{w}} \frac{2}{||\mathbf{w}||} \text{ subject to } \mathbf{w}^\top \mathbf{x}_i + b \begin{array}{ll} \geq 1 & \text{if } y_i = +1 \\ \leq -1 & \text{if } y_i = -1 \end{array} \text{ for } i = 1 \ldots N$$

- Or equivalently

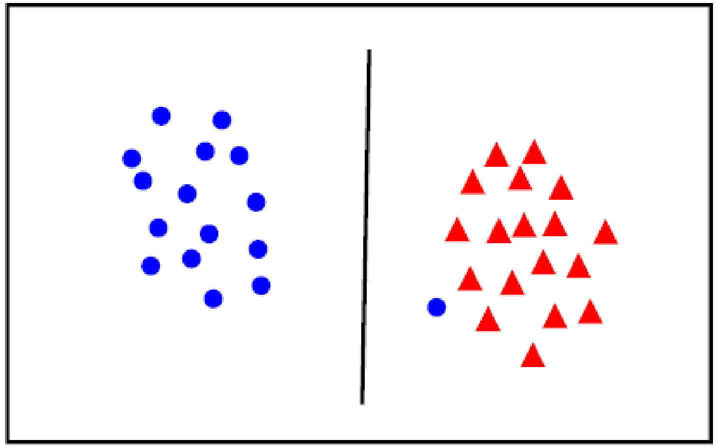
$$\min_{\mathbf{w}} ||\mathbf{w}||^2 \text{ subject to } y_i \left(\mathbf{w}^\top \mathbf{x}_i + b\right) \geq 1 \text{ for } i = 1 \ldots N$$

- This is a quadratic optimization problem subject to linear constraints and there is a unique minimum

Linear separability again: What is the best w?



• the points can be linearly separated but there is a very narrow margin



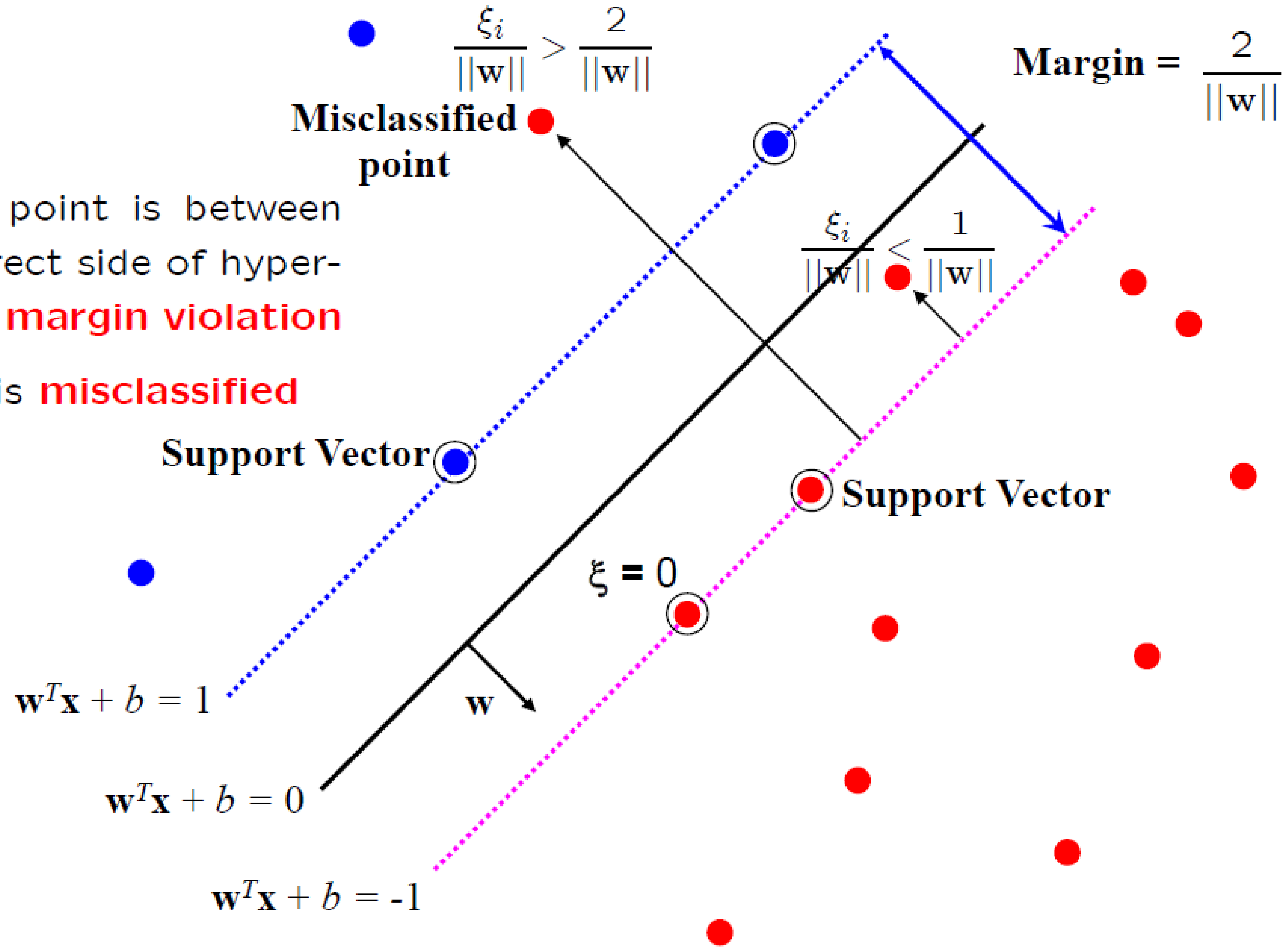
• but possibly the large margin solution is better, even though one constraint is violated

In general there is a trade off between the margin and the number of mistakes on the training data

Introduce "slack" variables

$$\xi_i \geq 0$$

- for $0 < \xi \leq 1$ point is between margin and correct side of hyper-plane. This is a **margin violation**
- for $\xi > 1$ point is **misclassified**



"Soft" margin solution

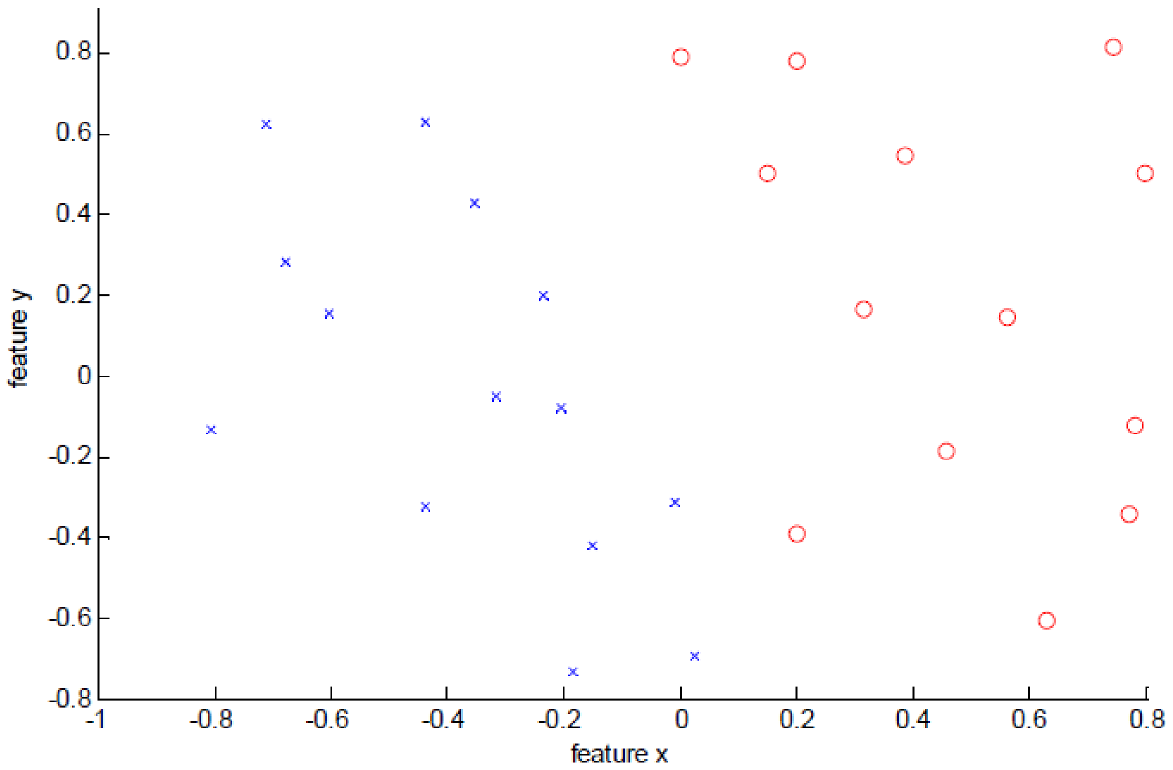
The optimization problem becomes

$$\min_{\mathbf{w}\in\mathbb{R}^d,\xi_i\in\mathbb{R}^+} ||\mathbf{w}||^2 + C\sum_i^N \xi_i$$

subject to

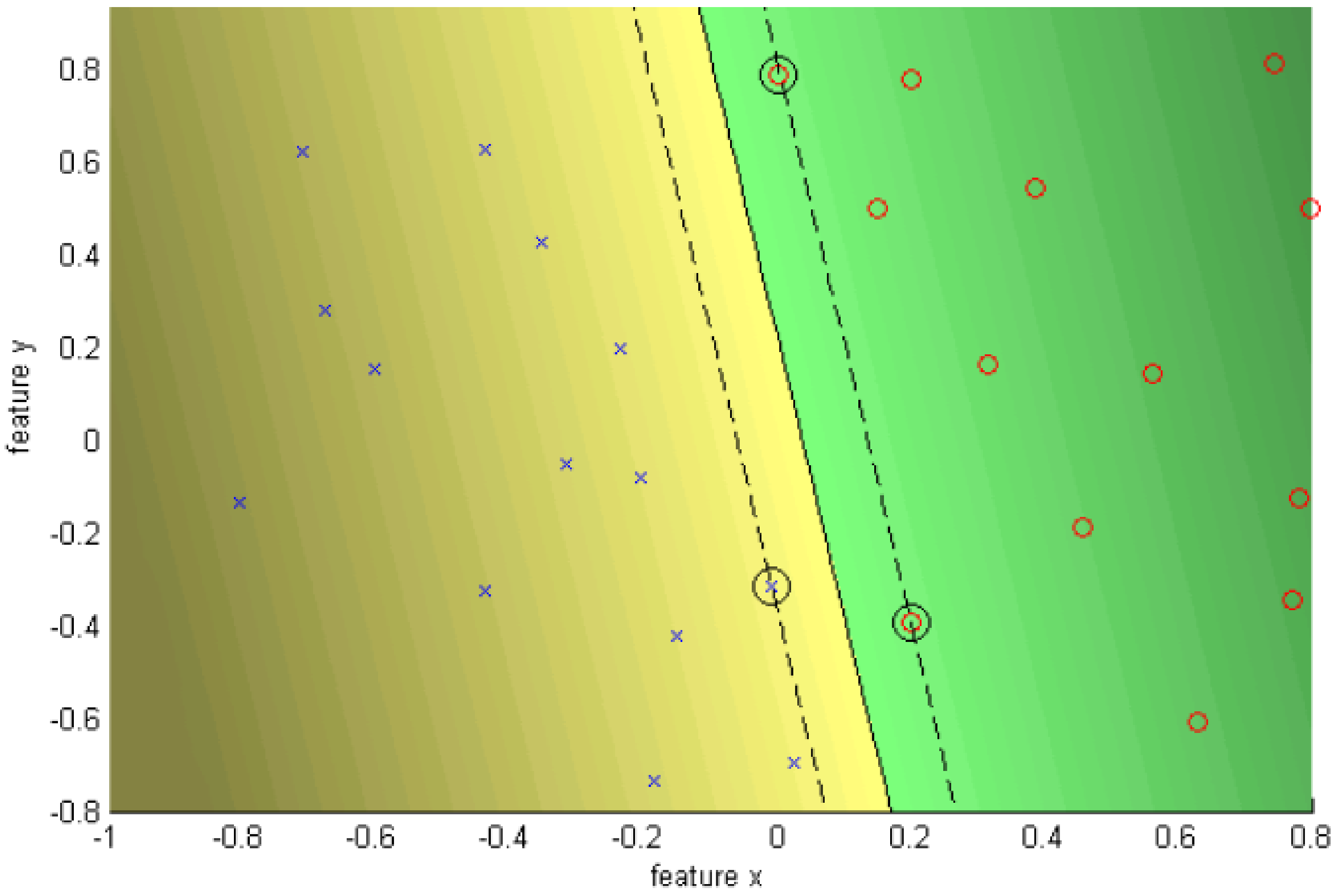
$$y_i\left(\mathbf{w}^\top \mathbf{x}_i + b\right) \geq 1 - \xi_i \text{ for } i = 1\ldots N$$

- Every constraint can be satisfied if ξ_i is sufficiently large
- C is a regularization parameter:
  - small C allows constraints to be easily ignored $\rightarrow$ large margin
  - large C makes constraints hard to ignore $\rightarrow$ narrow margin
  - $C = \infty$ enforces all constraints: hard margin
- This is still a quadratic optimization problem and there is a unique minimum. Note, there is only one parameter, C.

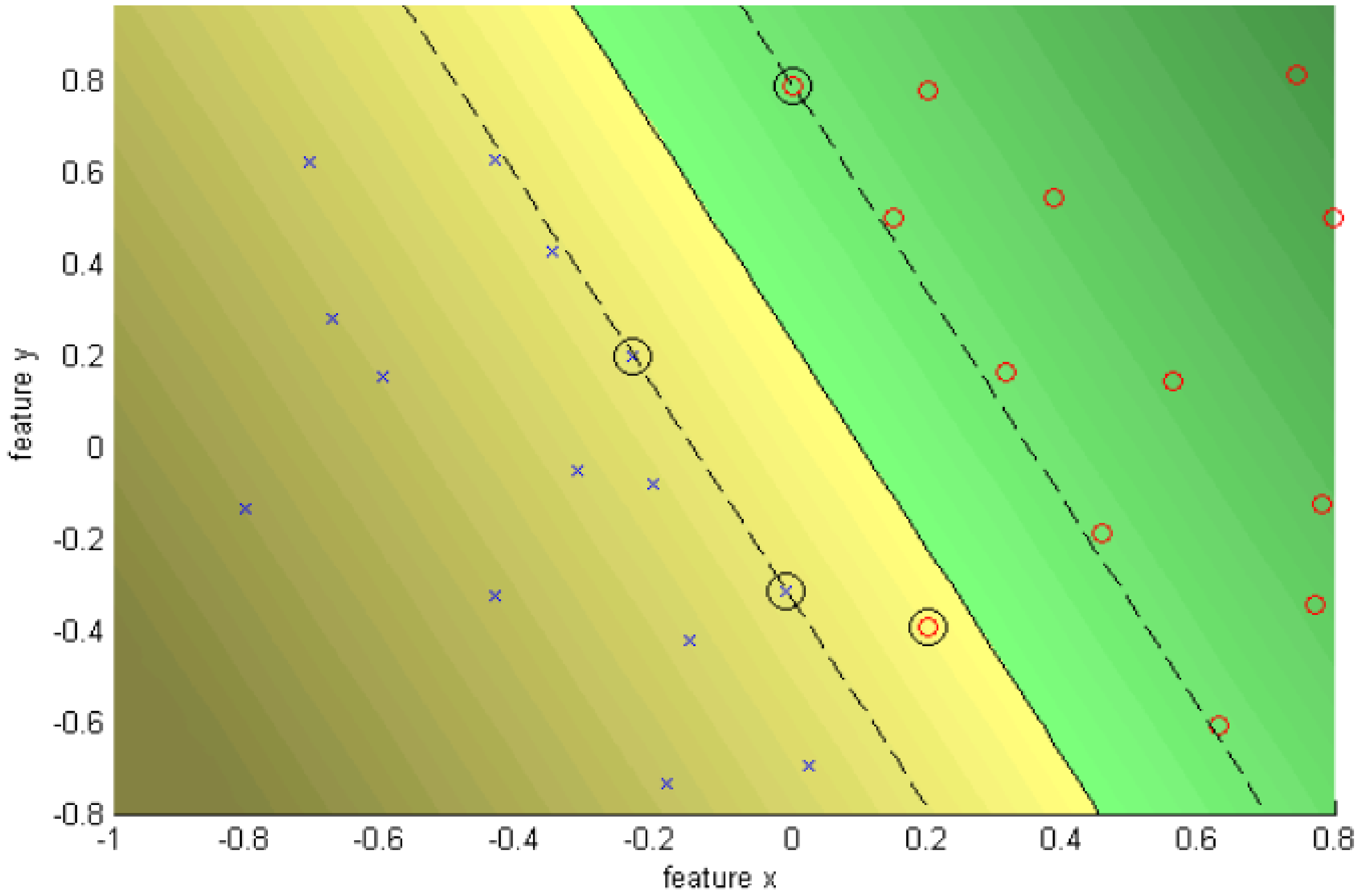


- data is linearly separable
- but only with a narrow margin

C = Infinity   hard margin



C = 10   soft margin



Optimization

Learning an SVM has been formulated as a constrained optimization problem over $\mathbf{w}$ and ξ

$$\min_{\mathbf{w}\in\mathbb{R}^d,\xi_i\in\mathbb{R}^+} ||\mathbf{w}||^2 + C\sum_i^N \xi_i \text{ subject to } y_i\left(\mathbf{w}^\top\mathbf{x}_i + b\right) \geq 1 - \xi_i \text{ for } i = 1\ldots N$$

The constraint $y_i\left(\mathbf{w}^\top\mathbf{x}_i + b\right) \geq 1 - \xi_i$, can be written more concisely as

$$y_i f(\mathbf{x}_i) \geq 1 - \xi_i$$

which, together with $\xi_i \geq 0$, is equivalent to

$$\xi_i = \max\left(0, 1 - y_i f(\mathbf{x}_i)\right)$$

Hence the learning problem is equivalent to the unconstrained optimization problem over $\mathbf{w}$

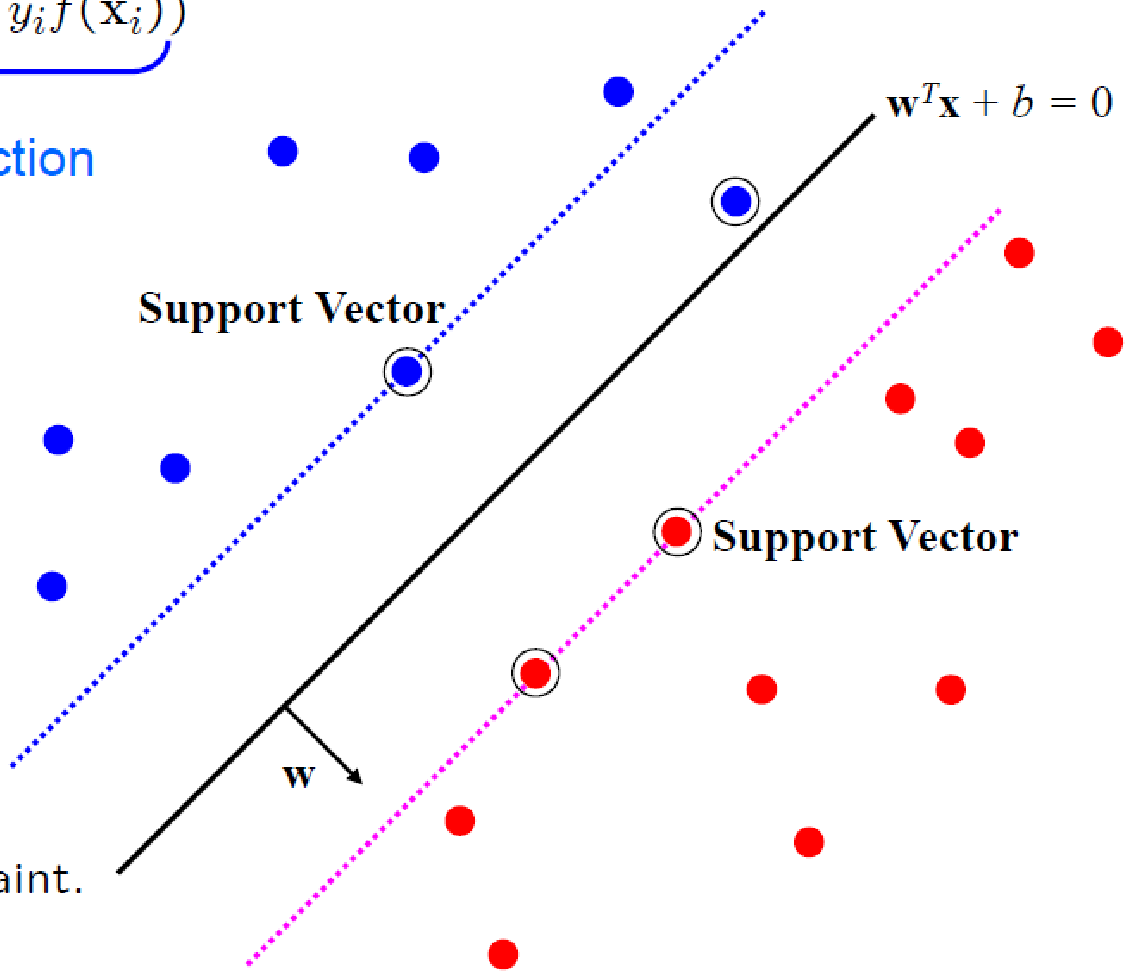
$$\min_{\mathbf{w}\in\mathbb{R}^d} \underbrace{||\mathbf{w}||^2}_{\text{regularization}} + C\sum_i^N \underbrace{\max\left(0, 1 - y_i f(\mathbf{x}_i)\right)}_{\text{loss function}}$$

Loss function

$$\min_{\mathbf{w}\in\mathbb{R}^d} ||\mathbf{w}||^2 + C\sum_i^N \underbrace{\max(0, 1 - y_i f(\mathbf{x}_i))}_{\text{loss function}}$$

Points are in three categories:

1. $y_i f(x_i) > 1$
   Point is outside margin.
   No contribution to loss
2. $y_i f(x_i) = 1$
   Point is on margin.
   No contribution to loss.
   As in hard margin case.
3. $y_i f(x_i) < 1$
   Point violates margin constraint.
   Contributes to loss



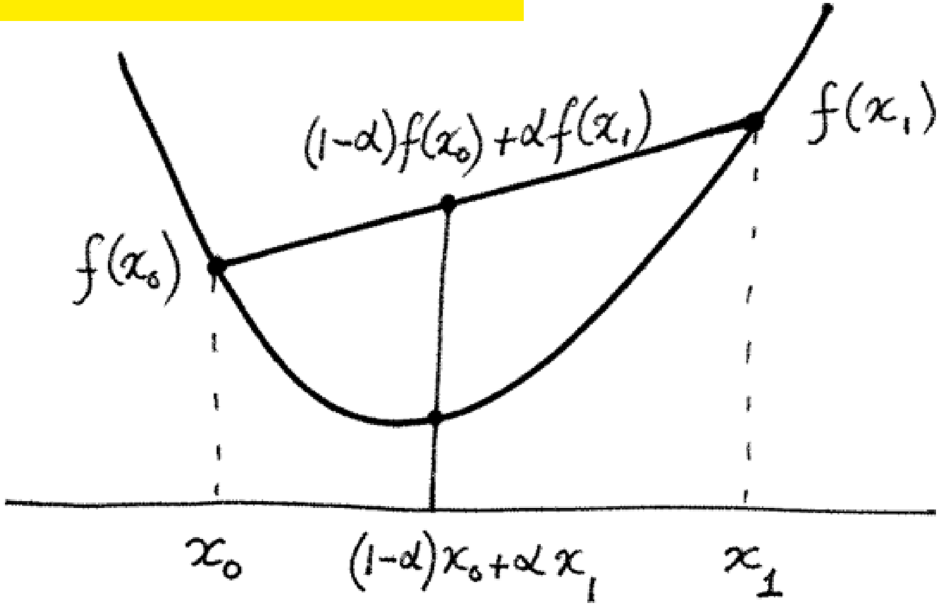
Convex functions

D – a domain in $\mathbb{R}^n$.

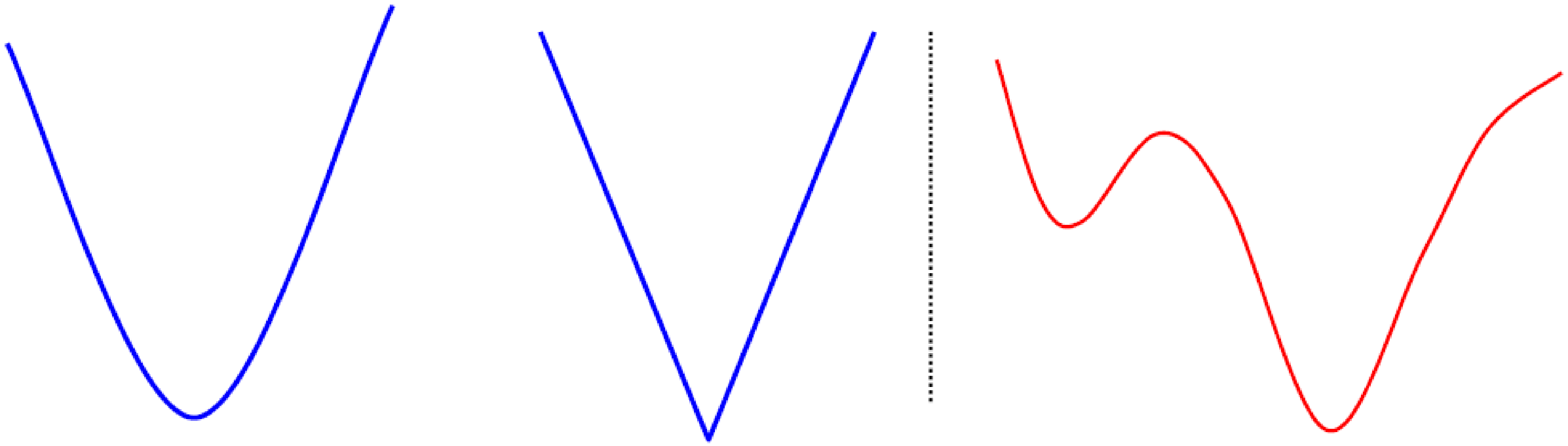
A convex function $f : D \rightarrow \mathbb{R}$ is one that satisfies, for any $\mathbf{x}_0$ and $\mathbf{x}_1$ in D:

$$f((1-\alpha)\mathbf{x}_0 + \alpha\mathbf{x}_1) \leq (1-\alpha)f(\mathbf{x}_0) + \alpha f(\mathbf{x}_1) \ .$$

Line joining $(\mathbf{x}_0, f(\mathbf{x}_0))$ and $(\mathbf{x}_1, f(\mathbf{x}_1))$ lies above the function graph.



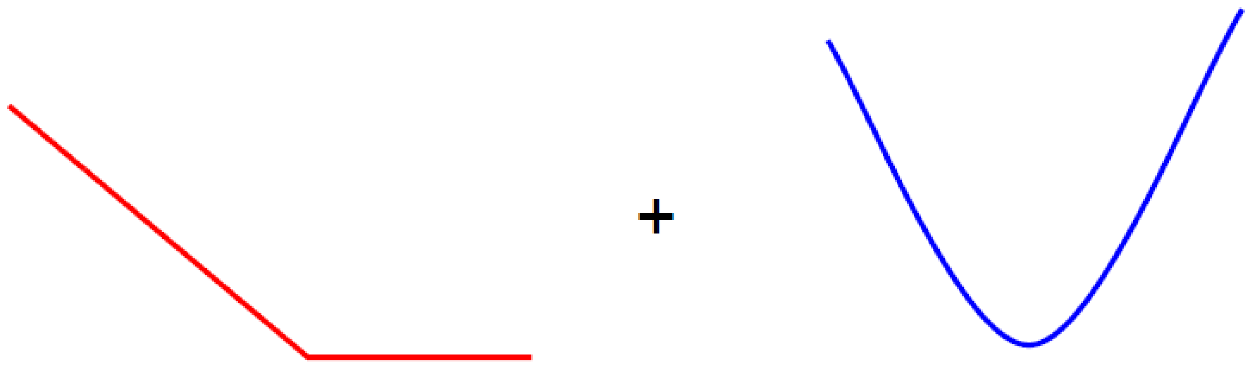
Convex function examples



convex

Not convex

A non-negative sum of convex functions is convex



SVM

$$\min_{\mathbf{w}\in\mathbb{R}^d} C \sum_i^N \max\left(0, 1 - y_i f(\mathbf{x}_i)\right) + ||\mathbf{w}||^2 \qquad \text{convex}$$

Gradient (or steepest) descent algorithm for SVM

To minimize a cost function $\mathcal{C}(\mathbf{w})$ use the iterative update

$$\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t - \eta_t \nabla_{\mathbf{w}} \mathcal{C}(\mathbf{w}_t)$$

where η is the learning rate.

First, rewrite the optimization problem as an average

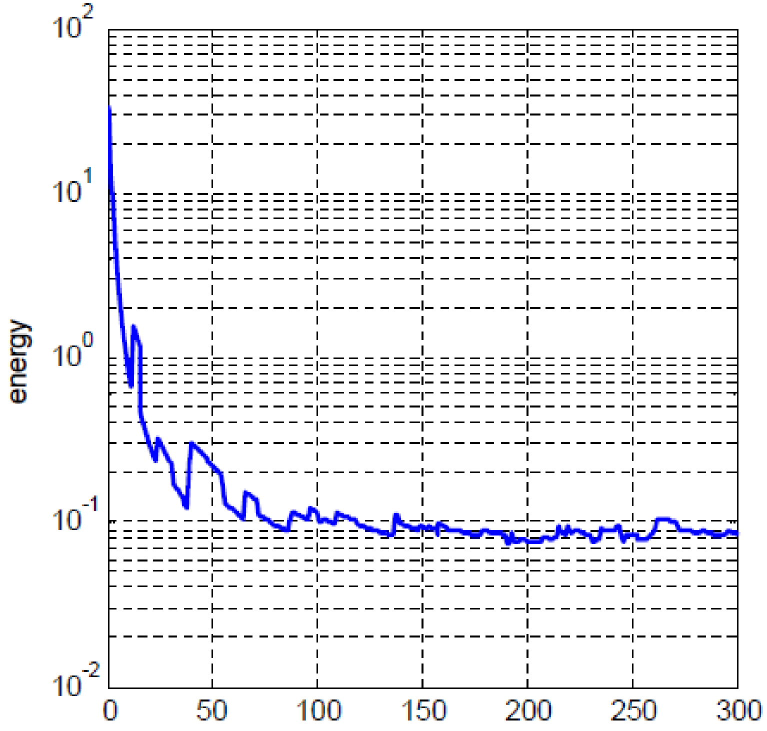
$$\begin{aligned}
\min_{\mathbf{w}} \mathcal{C}(\mathbf{w}) &= \frac{\lambda}{2}||\mathbf{w}||^2 + \frac{1}{N}\sum_i^N \max(0, 1 - y_i f(\mathbf{x}_i)) \\
&= \frac{1}{N}\sum_i^N \left(\frac{\lambda}{2}||\mathbf{w}||^2 + \max(0, 1 - y_i f(\mathbf{x}_i))\right)
\end{aligned}$$

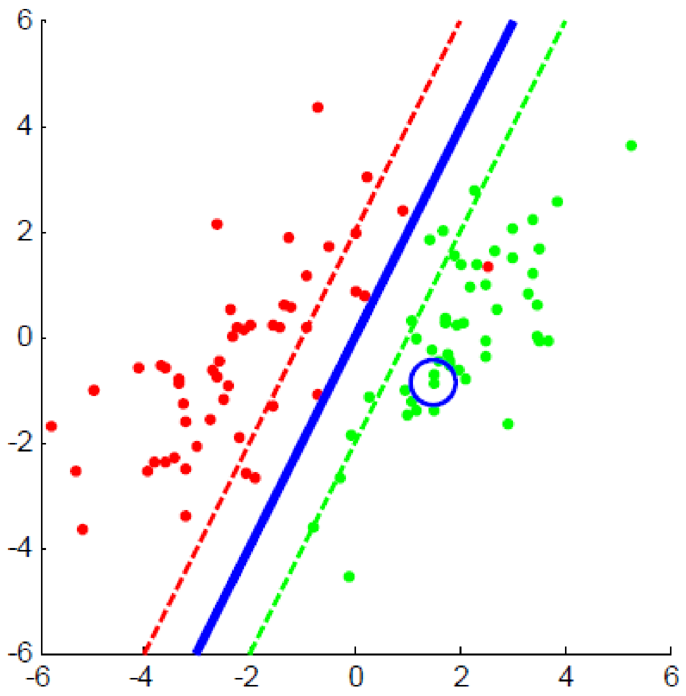
(with $\lambda = 2/(NC)$ up to an overall scale of the problem) and $f(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + b$

Because the hinge loss is not differentiable, a sub-gradient is computed

Pegasos – Stochastic Gradient Descent Algorithm

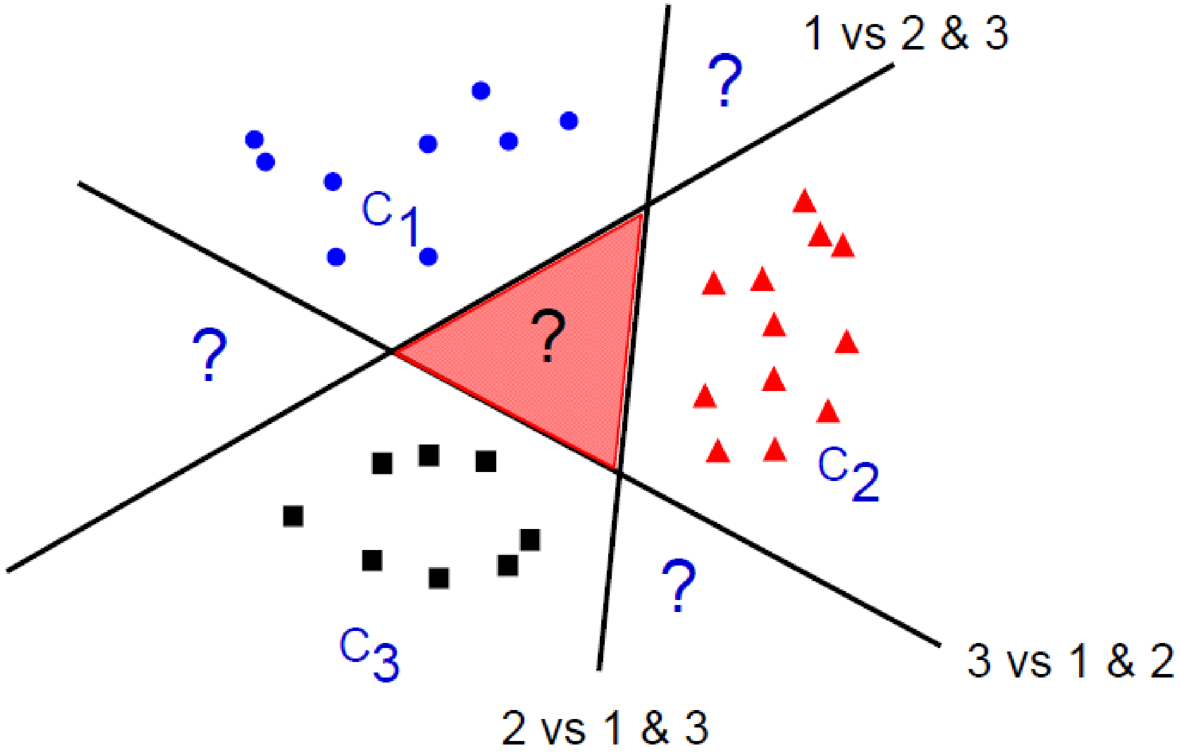
Randomly sample from the training data





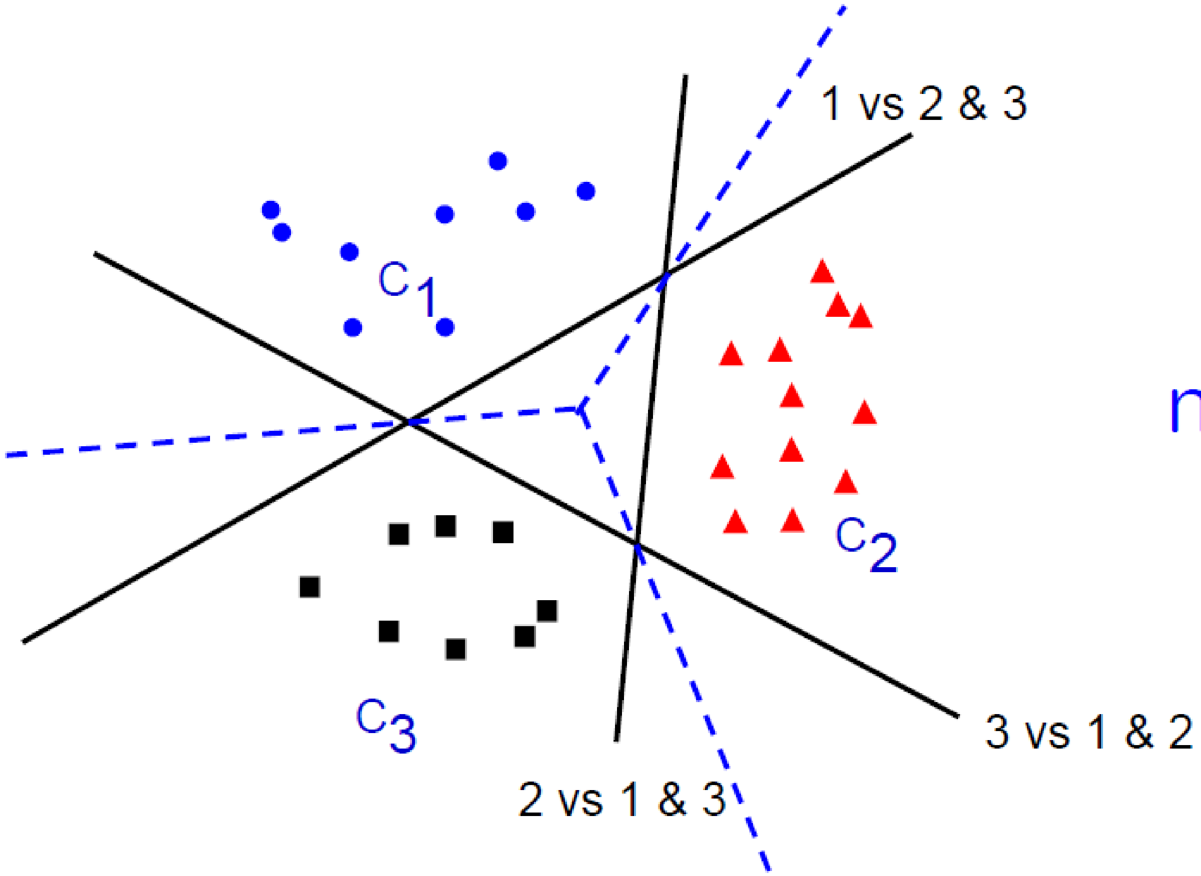
M-Class Classifiers

- Learn: K two-class 1-vs-the-rest classifiers $f_k(\mathbf{x})$



Build from binary classifiers continued

- Learn: K two-class 1 vs the rest classifiers $f_k(\mathbf{x})$
- Classification: choose class with most positive score



$$\max_k f_k(\mathbf{x})$$

Build from binary classifiers continued

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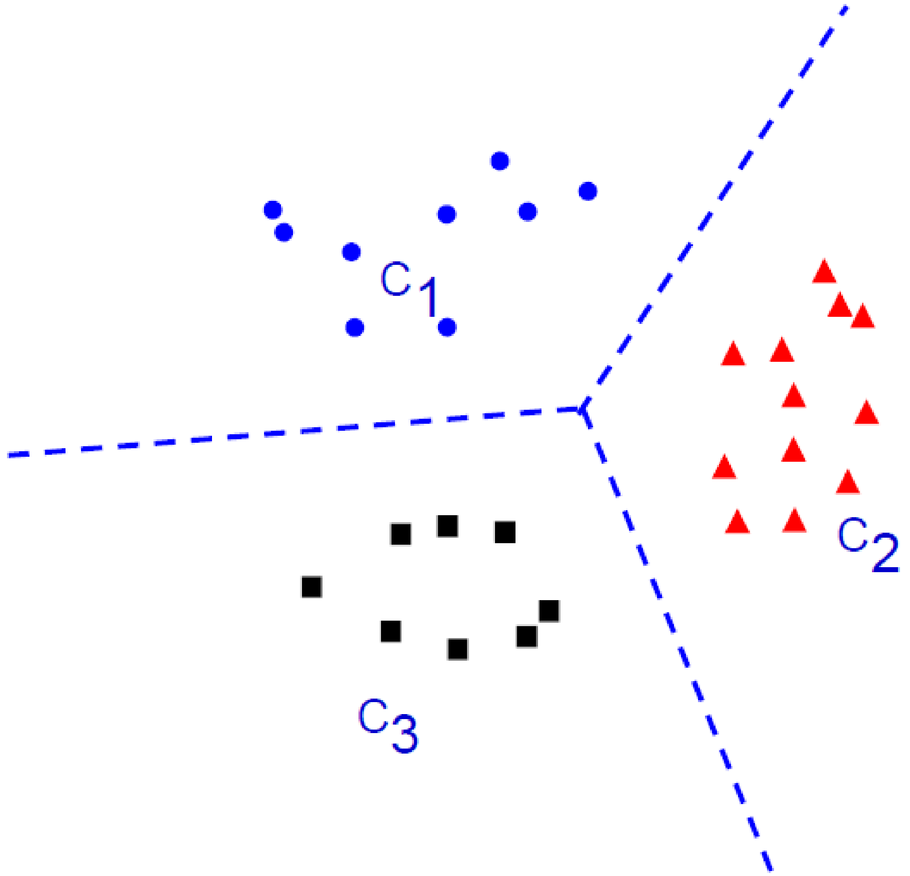

$$\max_k f_k(\mathbf{x})$$

Next Lecture

- We will see that the SVM can be written as a sum over the support vectors

$$f(x) = \sum_i \alpha_i y_i (\mathbf{x}_i{}^\top \mathbf{x}) + b$$

support vectors

- Handling Nonlinearly separable data via Kernelized SVMs
- Kernel Spaces
- RBF kernels